On a Rational Approximation of the Kernel Function in the Integral Equation for the Heating Function

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On a Rational Approximation of the Kernel Function in the Integral Equation for the Heating Function.

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Abstract: The computation method for the kernel function in the integral equation for the heating rate is studied. It is shown that the kernel function can be expressed in terms of the transmission function and a few kinds of analytic functions on the assumption of the random array of a finite number of spectral lines (quasi-random model), and that those analytic functions can be approximated in the rational expressions with small errors.

1. Introduction

The radiative temperature change in the upper atmosphere is caused by a little fluctuation of the radiative net flux because of its small heat capacity. Hence, for the purpose of estimating the heating rate in the upper atmosphere, it seems more appropriate to use the integral equation for the heating function than the equation of transfer for the radiative flux, because in the latter equation the exact transmission function, which is very difficult to evaluate, is needed.

The kernel function of the integral equation has too complicated form to be computed directly. In the upper atmosphere, however, the spectral lines are as narrow that the effect of line overlap can be ignored. In this case, the kernel function can be expressed in terms of analytic functions having different forms according to the spectral line profiles, and the difficulty in the integration over frequency is avoided.

In this study, in order to simplify the computation of the kernel function furthermore, and to reduce the computer time, we have represented the analytic functions in the rational expressions within a minimum error in Chebyshev's meaning. (Minimax Approximation)

2. The integral equation for the heating function.

The equation for the heating rates in the upper atmosphere due to the i-th spectral interval in the 15 μ carbondioxide bands is given by (Curtis and Goody, 1956),

$$H_i(z)=\int_{K_i^{(1)}=0}^{1}\{J_i(z')-J_i(z)\}dK_i^{(1)}+\int_{K_i^{(2)}=0}^{1}\{J_i(z')-J_i(z)\}dK_i^{(2)} \tag{1}$$

and

$$K_i(z',z)=\left(\int_i e_\nu(z)d\nu\right)^{-1}\int_i e_\nu(z)\,E_2\{|\tau_\nu(z',\infty)-\tau_\nu(z,\infty)|\}d\nu \tag{2}$$

where z ; altitude from the earth surface,

H_i; heating function for the i-th spectral interval,

J_i : source function for the i-th spectral interval,

e_ν : extinction coefficient at frequency ν,

τ_ν ; optical depth from the top of the atmosphere,

and $K_i^{(1)}$ and $K_i^{(2)}$ are defined for $z'<z$ and $z'>z$, respectively. The i-th spectral interval is assumed to be so narrow that the source function J_ν can be replaced by its average value, but wide enough to contain many spectral lines. The function E_2 is the second order exponential integral defined by,

$$E_2(x) = \int_0^1 e^{-x/\mu}\, d\mu$$

The temperature change $(\partial\vartheta/\partial t)_z$ at z can be expressed in terms of the heating function as

$$C_p w \cdot \left(\frac{\partial\vartheta}{\partial t}\right)_z = 2\pi \sum_i H_i(z) \int_i e_\nu(z)\, d\nu \tag{3}$$

where C_p is the heat capacity at constant pressure, and w is the mixing ratio of the absrobing matter. The summation extends over all frequency intervals.

To estimate the equation (1), we devide the atmosphere into datum levels which are numbered by consecutive integers (r, s). Then using a suitable formula for numerical quadrature, the integration can be transformed into the linear system given by,

$$H_i^{(r)} = \sum_s A_i^{(r,s)} J_i^{(s)} \tag{4}$$

where $A_i^{(r,s)}$'s are the weights appropriate to the quadrature formula.

The exact solution may be obtained in this way, but an approximate solution for the upper atmosphere can simply be obtained as follows. At the low pressure, the term representing the cooling to space tends to dominate all others (Curtis and Goody, 1956). Then the heating function (1) can be approximated by

$$H_i(z) = -J_i(z) K_i^{(2)}(\infty, z) \tag{5}$$

Here the source function $J_i(z)$ is given by,

$$J_i(z) = B_i(z) + \frac{\lambda_i(z)}{\phi_i(z)} H_i(z) \tag{6}$$

where λ_i and ϕ_i are respectively the collisional and radiative life time of the vibrationally excited state. In equations (5) and (6), the spectral interval (i) must be sufficiently wide to embrace the whole of a vibration-rotation band. Substituting (6) into (5), we have

$$H_i(z) = -K_i^{(2)}(\infty, z)\, B_i(z) \left\{1 + \frac{\lambda_i(z)}{\phi_i(z)} K_i^{(2)}(\infty, z)\right\}^{-1} \tag{7}$$

This equation reveals the important role of the function $K_i^{(2)}(\infty, z)$ on the cooling rate in the upper atmosphere.

3. Computation of the kernel function

For a spectral interval containing many lines, the numerical integration of the equation (2) is so time-consuming that we adopt an approximation using the band model approach.

We shall assume that the atmosphere is homogeneous, where the mixing ratio of absorbing matter and the pressure are constant, and that the i-th spectral interval contains N lines. The kernel function is then written in the form

$$K_i(z', z) = \int_0^1 K_i(z', z, \mu)\, d\mu \tag{8}$$

and

$$K_i(z', z, \mu) = \frac{\sum_{j=1}^{N} \int_i k_{\nu j} \prod_{l=1}^{N} \exp(-a/\mu \cdot k_{\nu l})\, d\nu}{\sum_{j=1}^{N} \int_i k_{\nu j}\, d\nu} \tag{9}$$

where $k_{\nu l}$; absorption coefficient at frequency ν for the l-th line,

a ; amount of absorbing matter,

μ ; direction cosine of a zenith angle.

From the assumption of a homogeneous atmosphere the band contour does not change along the absorption path. Hence the kernel function $K_i(z', z)$ is symmetric with respect to z and z'. Using the random model of Goody (1964) for the mean transmission, the kernel function averaged over the interval is given by,

$$\bar{K}_i(z', z, \mu) = \frac{\sum_{j=1}^{N} \int_i k_{\nu j} \exp(-a/\mu \cdot k_{\nu j})\, d\nu \prod_{l \neq j} \frac{1}{N} \int_i \frac{d\nu}{\delta} \exp(-a/\mu \cdot k_{\nu l})}{\sum_{j=1}^{N} \int_i k_{\nu j}\, d\nu} \tag{10}$$

Correspondingly the average transmissivity for the same interval is given by,

$$\bar{T}_i(a, \mu) = \prod_{j=1}^{N} \frac{1}{N} \int_i \frac{d\nu}{\delta} \exp(-a/\mu \cdot k_{\nu j}) \tag{11}$$

where δ is the mean line spacing. When the interval contains many lines, eq. (10) is written, by using eq. (11), in the form

$$\bar{K}_i(z', z, \mu) = \bar{T}_i(a, \mu) \cdot \sum_{j=1}^{N} L(j; z) \cdot T(j; z', z, \mu) \tag{12}$$

where

$$T(j; z', z, \mu) = \int_{-\infty}^{+\infty} f_\nu(j; z) \cdot \exp(-a/\mu \cdot k_{\nu j})\, d\nu \tag{13}$$

$$L(j; z) = \frac{S_j(z)}{\sum_j S_j(z)}$$

S_j; strength of the j-th line,

f_ν; line profile function.

The function $T(j; z', z, \mu)$ gives the probability that a photon emitted at level z in the direction μ at any frequency in the j-th line escapes to level z'. This function is called the line escape function (Dickinson, 1972).

For the kernel function (8) averaged over the zenith angle, the factor γ is introduced, which has similar meaning to the diffusivity factor used in the transmission function for the diffused radiative flux.

Then the function (8) is written as

$$\bar{K}_i(z', z) = \bar{T}_i(\gamma a) \cdot \sum_{j=1}^{N} L(j; z) \cdot T(j; z', z) \tag{14}$$

where

$$T(j; z', z) = \int_{-\infty}^{+\infty} f_\nu(j; z) \cdot E_2(ak_{\nu j})\, d\nu \tag{15}$$

The value of γ can be decided from the leastsquares fit of the form $E_2(x) \simeq e^{-\gamma x}$. The value of 2.258893 is obtained as the most plausible value of γ.

The comparison of the behavior of the Elssaser function $E(y, \gamma u)$ and that of the function $\bar{E}(y, u)$ defined by,

$$\bar{E}(y, u) = \int_0^1 E(y, u/\mu)\, d\mu$$

is given in Fig. 1. Here γ is a numerical factor described above, u is a half optical depth at the line center, and y is a Lorentz half width devided by the mean line spacing. The mean value of u does not exceed 10^4 in the real atmosphere.

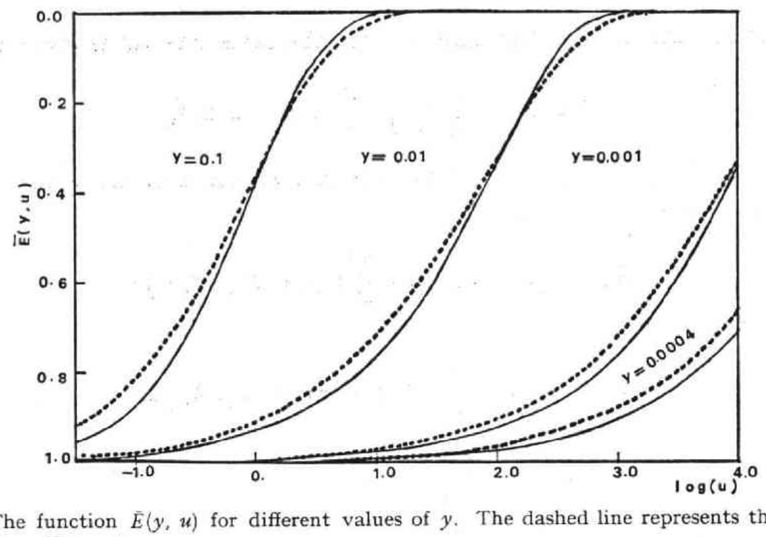

Fig. 1 The function $\bar{E}(y, u)$ for different values of y. The dashed line represents the Elssaser function $E(y, \gamma u)$.

For the real inhomogeneous atmosphere, it seems appropriate to use the Curtis-Godson approximation (Goody, 1964), or the improved C.G. approximation by Yamamoto *et al.* (1972), to replace the nonhomogeneous path by the homogeneous one. In this case, the kernel function becomes asymetric with respect to z and z'.

4. Line escape functions and their rational approximations.

The escape functions $T(j; z' z, \mu)$ and $T(j; z', z)$ for the homogeneous path can be rewritten using the non-dimensional quantity τ and the dimensionless function $\phi(x)$ in the form

$$T(j; z', z, \mu) = \int_{-\infty}^{+\infty} \phi(x) \exp\{-\tau\phi(x)\} dx \tag{16}$$

$$\equiv R(\tau)$$

$$T(j; z', z) = \int_{-\infty}^{+\infty} \phi(x)\, E_2\{\tau\phi(x)\} dx \tag{17}$$

$$\equiv T(\tau)$$

where

$$\phi(x) = \frac{1}{\pi}\frac{1}{1+x^2}, \quad \tau = \frac{su}{a_L} \qquad \text{for the Lorentz profile,}$$

$$\phi(x) = \frac{1}{\sqrt{\pi}} e^{-x^2}, \quad \tau = \frac{su}{a_D} \qquad \text{for the Doppler Profile,}$$

and

$$\phi(x) = \frac{d}{\pi^{3/2}} \int_{-\infty}^{+\infty} \frac{e^{-t^2}}{d^2+(x-t)^2} dt,$$

$$\tau = \frac{su}{a_D}\sqrt{\ln 2}, \quad d = \frac{a_L}{a_D}\sqrt{\ln 2} \quad \text{for the Voigt profile.}$$

Here a_L and a_D are the Lorentz and Doppler half widths, and the amount u must be taken as a/μ or a for the function $R(\tau)$ or $T(\tau)$, respectively. If necessary, we shall denote the Doppler, Lorentz and Voigt escape functions by T_D, T_L and T_V.

The Voigt profile tends to the Lorentz and Doppler profiles in the limits of $d \to \infty$ and $d \to 0$, respectively. Fig. 2 shows the Voigt escape function T_V averaged over the zenith angle as a function of τ for several values of d. The curve for $d=0$ just approaches the Doppler escape function. As d or τ increases, the Voigt escape function approaches the Lorentz escape function; the value of the Lorentz escape function is proportional to $1/\sqrt{\tau}$ (the square root law).

For the non-homogeneous path, using the Curtis-Godson approximation, the Lorentz escape functions are given by

$$R_L(z', z) = \int_{-\infty}^{+\infty} \psi(x, q) \exp\{-\tau\phi(x)\} dx \tag{18}$$

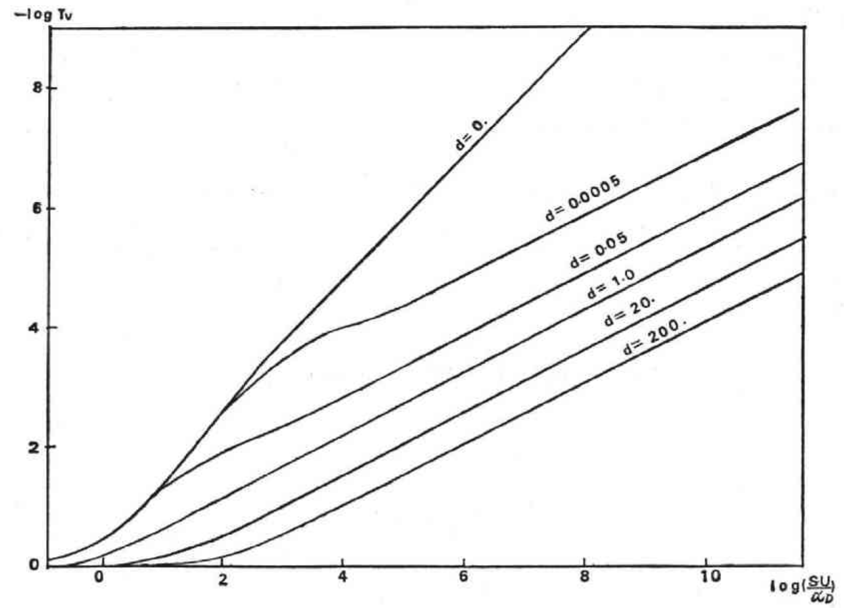

Fig. 2 Voigt escape function as a function of $\tau(=su/\alpha_0)$ for different values of d.

$$T_L(z', z) = \int_{-\infty}^{+\infty} \psi(x, q)\, E_2\{\tau\phi(x)\}dx \tag{19}$$

where

$$\psi(x, q) = \frac{1}{\pi}\frac{q}{q^2+x^2}$$

$$q = \alpha_L(z)/\tilde{\alpha}_L\,, \qquad (0 \leq q \lesssim 1)$$

$$\tau = \tilde{s}u/\tilde{\alpha}_L$$

$\tilde{\alpha}_L$; effective Lorentz width appropriate to Curtis-Godson approximation,

$\tilde{S}$; effective line strength.

We can expand the function $\psi(x, q)$ in Taylor's series with respects to $(q-1)$ in the form

$$\psi(x, q) = \phi(x) + \{\phi(x) - 2\pi\phi^2(x)\}(q-1) + \cdots \tag{20}$$

Neglecting the terms higher than second order, we have

$$R_L(z', z) \simeq qR_L(\tau) + (1-q)\, S_L(\tau) \tag{21}$$

and

$$T_L(z', z) \simeq qT_L(\tau) + (1-q)\, U_L(\tau) \tag{22}$$

where functions $S_L(\tau)$ and $U_L(\tau)$ are defined by

$$S_L(\tau) = 2\pi\int_{-\infty}^{+\infty} \phi^2(x)\exp\{-\tau\phi(x)\}\,dx \tag{23}$$

and

$$U_L(\tau) = 2\pi\int_{-\infty}^{+\infty} \phi^2(x)\, E_2\{\tau\phi(x)\}dx \tag{24}$$

It is easy to show that the functions $R_L(\tau)$ and $S_L(\tau)$ can be expressed in terms of modified Bessel functions of the first kind with imaginary arguments in the form

$$S_L(\tau) = \exp(-\tau/2\pi)\{I_0(\tau/2\pi) - I_1(\tau/2\pi)\} \tag{25}$$

and

$$R_L(\tau) = \exp(-\tau/2\pi)\cdot I_0(\tau/2\pi) \tag{26}$$

From (21), the function $R_L(z'\ z)$ is expressed analytically in terms of the modified Bessel functions.

For the other functions such as T_L, T_D and R_D we can approximate these functions by the rational expressions, of which unknown coefficients are determined to achieve best fit in Chebyshev's meaning to those computed exactly by numerical calculation. For the function T_L, for example, the asymptotic expansion of the function as $\tau\to\infty$,

$$T_L(\tau) \sim \frac{2}{3\sqrt{\tau}}\left\{1 + \frac{3\pi}{20}\tau^{-1} + \frac{27\pi^2}{224}\tau^{-2} + \cdots\right\},$$

leads us to the following rational expression

$$T_L{}^*(\tau) = \frac{2}{3\sqrt{\tau}}\cdot\frac{1+a_1\left(\frac{2\pi}{\tau}\right)+a_2\left(\frac{2\pi}{\tau}\right)^2+a_3\left(\frac{2\pi}{\tau}\right)^3}{1+b_1\left(\frac{2\pi}{\tau}\right)+b_2\left(\frac{2\pi}{\tau}\right)^2+b_3\left(\frac{2\pi}{\tau}\right)^3}, \quad \text{for} \quad 1 \leq \frac{\tau}{2\pi} < \infty$$

From the best fit in Chebyshev's meaning, the numerical coefficients are determined as follows;

$$a_1 = -0.7702589641, \qquad a_2 = 1.142758339, \qquad a_3 = 0.7982904562,$$
$$b_1 = -0.8466871993, \qquad b_2 = 1.199808496, \qquad b_3 = 0.6055112081.$$

The relative error included in this approximate expression does not exceed 0.0027%, which is of sufficiently accurate for all most of our purpose (Fig. 3). Similar expressions are also derived for other functions. The forms of rational expansion, values of

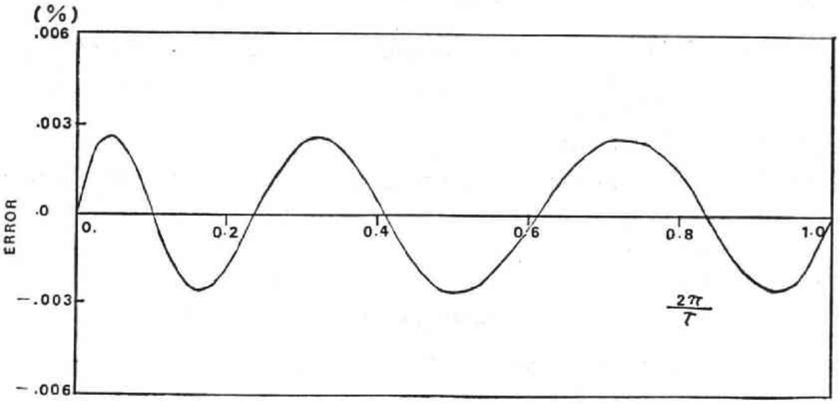

Fig. 3 Relative error of the approximation $T_L{}^*$ for T_L.

coefficients and maximum relative error are listed in the following

$$R_D^*(\tau) = \frac{1}{\tau\sqrt{\xi}} \cdot \frac{1+a_1\xi^{-1}+a_2\xi^{-2}}{1+b_1\xi^{-1}+b_2\xi^{-2}+b_3\xi^{-3}}$$

$[4 \leq \xi < \infty]$ $\qquad \xi = ln\,(\tau/\sqrt{\pi}\,)$

$a_1 = 1.808457494$, $\quad a_2 = -1.882979115$,

$b_1 = 2.096980867$, $\quad b_2 = -2.013933646$, $\quad b_3 = 0.5644188381$

maximum relative error $<0.000045(\%)$

$$R_D^*(\tau) = \{1+a_1\xi+a_2\xi^2+a_3\xi^3+a_4\xi^4+a_5\xi^5+a_6\xi^6\}^{-4}$$

$[0 \leq \xi \leq 10]$ $\qquad \xi = \tau/\sqrt{\pi}$

$a_1 = 0.1755752223$, $\quad a_2 = 0.8469700164\times 10^{-3}$,

$a_3 = -0.3116439059\times 10^{-3}$ $\quad a_4 = 0.2122223198\times 10^{-4}$,

$a_5 = 0.2836483344\times 10^{-7}$, $\quad a_6 = -0.3391766376\times 10^{-7}$

maximum relative error $<0.017(\%)$

$$T_D^*(\tau) = \frac{1}{2\tau\sqrt{\xi}} \cdot \frac{1+a_1\xi^{-1}+a_2\xi^{-2}+a_3\xi^{-3}+a_4\xi^{-4}}{1+b_1\xi^{-1}+b_2\xi^{-2}+b_3\xi^{-3}+b_4\xi^{-4}+b_5\xi^{-5}}$$

$[1 \leq \xi < \infty]$ $\qquad \xi = ln\,(\tau/\sqrt{\pi}\,)$

$a_1 = -2.207329622$, $\quad a_2 = 0.8134081926$, $\quad a_3 = 1.743554582$,

$a_4 = -0.2291426306$,

$b_1 = -1.672716397$, $\quad b_2 = -1.104080844$, $\quad b_3 = 4.612340109$,

$b_4 = -2.244275553$, $\quad b_5 = 0.7366034338$

maximum relative error $<0.0050(\%)$

$$S_L^*(\tau) = \frac{2\pi}{5\tau^{3/2}}\ \frac{1+a_1\xi^{-1}+a_2\xi^{-2}+a_3\xi^{-3}}{1+b_1\xi^{-1}+b_2\xi^{-2}+b_3\xi^{-3}}$$

$[1 \leq \xi < \infty]$ $\qquad \xi = \tau/4\pi$

$a_1 = -1.668691115$, $\quad a_2 = 1.198723603$, $\quad a_3 = 0.01266115873$

$b_1 = -1.804003394$, $\quad b_2 = 1.406195812$, $\quad b_3 = -0.1577689258$

maximum relative error <0.0044 $(\%)$.

Thus the line escape functions can be approximated by the corresponding rational expressions with sufficient accuracy. It is clear that the computer time is greately reduced by this approximation.

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